

1,3-Propanediol, diacetate
628-66-0 | DTXSID30211889

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 4.16×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.35×10^{-1}

Confidence level: 7.39×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Dimethyl glutarate

Measured: 3.30×10^{-12}

Predicted: 3.76×10^{-12}

Image not found

Dimethyl adipate

Measured: 8.40×10^{-12}

Predicted: 6.84×10^{-12}

Image not found

Dimethyl succinate

Measured: 1.40×10^{-12}

Predicted: 1.93×10^{-12}

Image not found

Ethyl 3-ethoxypropionate

Measured: 2.29×10^{-11}

Predicted: 1.63×10^{-11}

Image not found

2-Ethoxyethyl acetate

Measured: 1.30×10^{-11}

Predicted: 1.03×10^{-11}